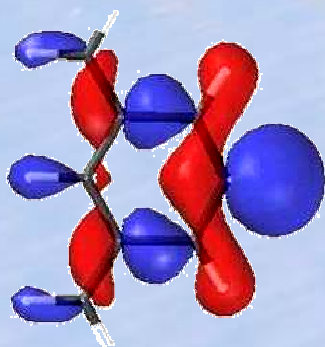


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Contrary to the standard orbital occupancy guidelines such as Aufbau principle or Hund's rule, three unpaired electrons are coupled antiferromagnetically in the 5-dehydro-*m*-xylylene (DMX) triradical, thus resulting in the **open-shell** doublet ground state. This electron arrangement is unprecedented for an organic molecule that does not include transition metals. Low-lying electronic states of DMX are shown on the right. Note that the closed-shell doublet (1^2B_2 state) in which electrons are distributed in accordance with the Aufbau principle is 2.5 eV above the ground state! Another likely candidate for the ground state, the quartet 1^4B_2 state, is 0.5 eV above the open-shell doublet, thus violating Hund's rule.



DMX was synthesized and experimentally characterized by our collaborators from Purdue University, Prof. P.G. Wenthold's group. The calculations were performed at USC by using the Spin-Flip method, a novel electronic structure approach which was recently developed in our group.

